



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2022 – 12:08 AM JST

PDB ID : 7DYJ  
Title : Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC  
Authors : Furuike, Y.; Akiyama, S.  
Deposited on : 2021-01-22  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

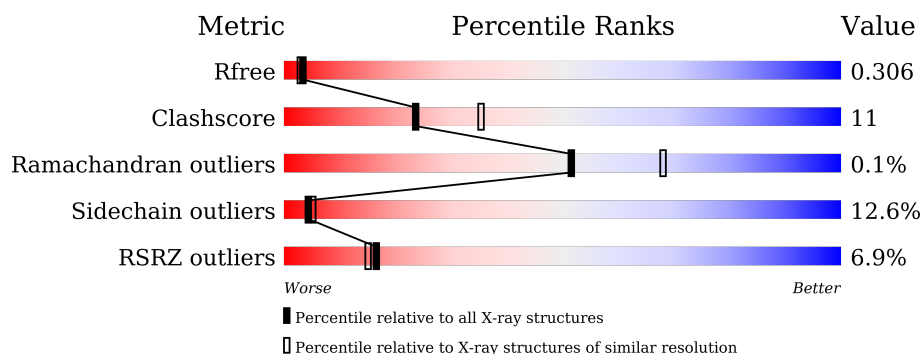
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>7%</div> <div>67%</div> <div>18%</div> <div>•</div> <div>12%</div> </div>
1	B	519	<div> <div>5%</div> <div>66%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition [i](#)

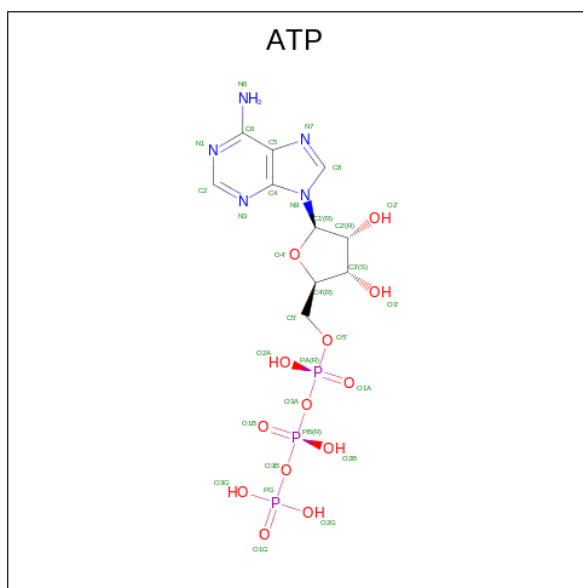
There are 4 unique types of molecules in this entry. The entry contains 6837 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	2	0
			3351	2125	583	629	14			
1	B	460	Total	C	N	O	S	0	2	0
			3302	2088	577	623	14			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mg 2	0	0
3	B	2	Total 2	Mg 2	0	0

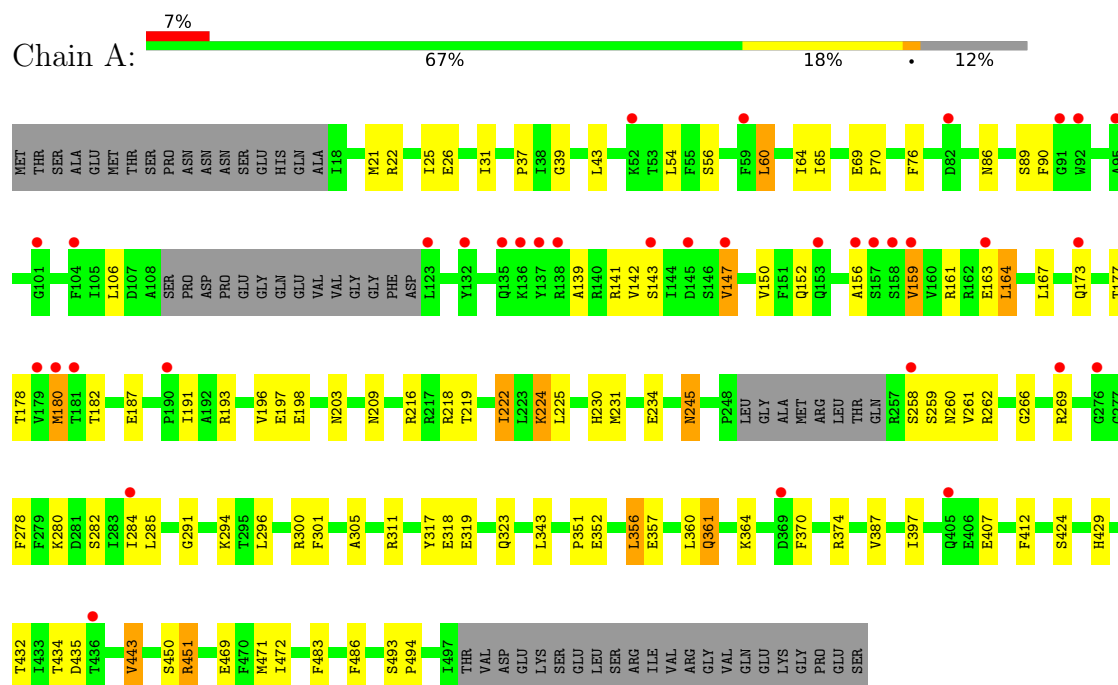
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	26	Total 26	O 26	0	0

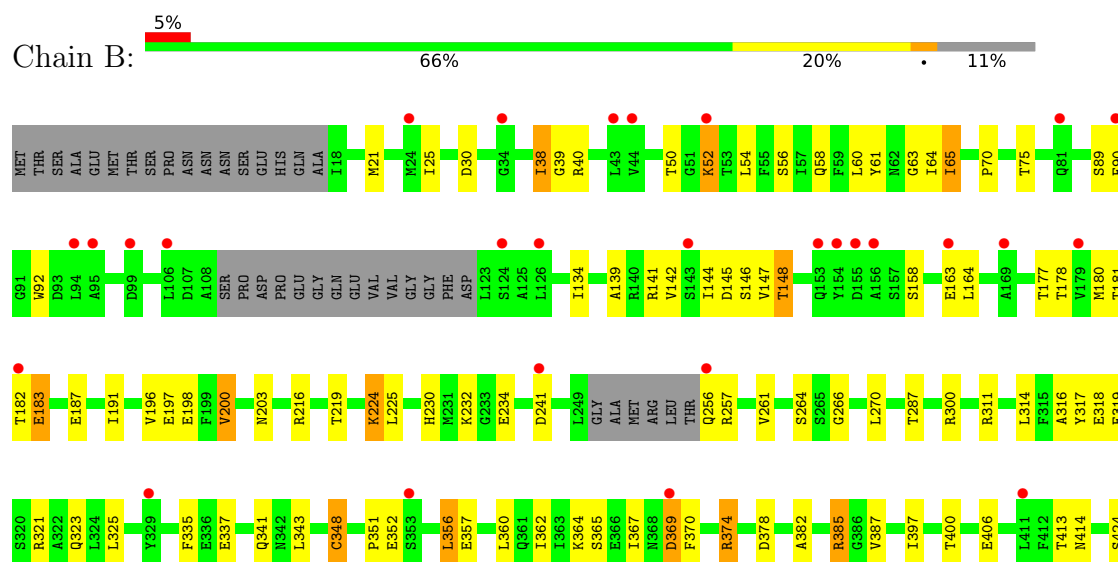
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Circadian clock protein kinase KaiC



#### • Molecule 1: Circadian clock protein kinase KaiC



H429	I430	S431	T432	I433	T434	D435	T436	I437	V443	M458	R459	H463	E469	F470	M471	F483	F486	I489	S493	P494	I497	THR	VAL	ASP	GLU	LYS	SER	GLU	LEU	SER	ARG	ILE	VAL	ARG	GLY	VAL	GLN	GLU	LYS	GLY	PRO	GLU	SER
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.58Å 94.58Å 179.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.29 – 2.40 29.27 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.29-2.40) 99.9 (29.27-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.267 , 0.310 0.268 , 0.306	Depositor DCC
$R_{free}$ test set	1681 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.931	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8311e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.68	0/3409	0.75	0/4624
1	B	0.69	0/3357	0.75	0/4560
All	All	0.68	0/6766	0.75	0/9184

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	256	GLN	Peptide
1	B	257	ARG	Peptide

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3351	0	3140	72	1
1	B	3302	0	3057	79	0
2	A	62	0	24	1	0
2	B	62	0	24	1	1
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	30	0	0	0	0
4	B	26	0	0	0	0
All	All	6837	0	6245	146	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLY:H	1:A:177:THR:HG22	1.34	0.92
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.59	0.84
1:A:429:HIS:O	1:A:432[A]:THR:HG22	1.84	0.77
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.67	0.77
1:B:70:PRO:HB2	1:B:139:ALA:HA	1.65	0.76
1:A:39:GLY:N	1:A:177:THR:HG22	2.01	0.75
1:A:21:MET:CE	1:A:177:THR:HG21	2.17	0.75
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.69	0.75
1:B:287:THR:HG22	1:B:414:ASN:HD22	1.52	0.74
1:B:356:LEU:CD2	1:B:387:VAL:HG11	2.18	0.72
1:A:152:GLN:O	1:B:158:SER:CB	2.37	0.72
1:B:164:LEU:HD11	1:B:180:MET:HE1	1.71	0.72
1:A:21:MET:HE3	1:A:177:THR:HG21	1.72	0.71
1:A:152:GLN:O	1:B:158:SER:HB3	1.90	0.71
1:B:316:ALA:O	1:B:348:CYS:HA	1.92	0.70
1:A:209:ASN:O	1:A:216:ARG:NH2	2.25	0.68
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.76	0.68
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.76	0.67
1:A:291:GLY:O	1:A:451:ARG:NH1	2.30	0.64
1:B:164:LEU:HD11	1:B:180:MET:CE	2.28	0.64
1:B:148:THR:HG22	1:B:182:THR:HA	1.80	0.64
1:B:317:TYR:HB3	1:B:351:PRO:HG3	1.79	0.64
1:A:86:ASN:OD1	1:B:40:ARG:NH1	2.32	0.63
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.81	0.62
1:B:134:ILE:HA	1:B:139:ALA:HB3	1.80	0.62
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:THR:CG2	1:B:182:THR:HA	2.30	0.61
1:A:152:GLN:O	1:B:158:SER:HB2	2.01	0.61
1:A:147:VAL:HG21	1:A:180:MET:HG2	1.81	0.60
1:B:483:PHE:HB3	1:B:486:PHE:CD2	2.36	0.60
1:A:31:ILE:HA	1:A:231:MET:SD	2.42	0.60
1:A:89:SER:OG	2:A:601:ATP:N6	2.32	0.58
1:B:61:TYR:O	1:B:65:ILE:HG23	2.02	0.58
1:A:26:GLU:HB2	1:A:245:ASN:HD22	1.68	0.58
1:B:21:MET:CE	1:B:177:THR:HG21	2.34	0.58
1:B:39:GLY:H	1:B:177:THR:HG22	1.68	0.58
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.39	0.57
1:B:429:HIS:O	1:B:432[A]:THR:HG22	2.04	0.57
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.86	0.57
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.35	0.57
1:B:58:GLN:HG2	1:B:92:TRP:CH2	2.40	0.56
1:B:225:LEU:HD12	1:B:230:HIS:HB3	1.87	0.56
1:A:245:ASN:OD1	1:A:361:GLN:NE2	2.39	0.56
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.41	0.56
1:B:264:SER:O	1:B:374:ARG:NH1	2.39	0.56
1:B:443:VAL:HG12	1:B:494:PRO:CD	2.37	0.55
1:A:219:THR:HB	1:A:234:GLU:HB3	1.89	0.55
1:B:58:GLN:CG	1:B:92:TRP:CH2	2.90	0.55
1:A:443:VAL:HG12	1:A:494:PRO:HD3	1.88	0.55
1:A:54:LEU:HD13	1:A:90:PHE:CZ	2.43	0.54
1:A:164:LEU:HD12	1:A:197:GLU:HA	1.89	0.54
1:B:39:GLY:N	1:B:177:THR:HG22	2.23	0.54
1:B:63:GLY:HA3	1:B:141:ARG:NE	2.23	0.53
1:B:147:VAL:O	1:B:147:VAL:HG12	2.08	0.52
1:A:280:LYS:HD3	1:A:280:LYS:C	2.30	0.52
1:B:142:VAL:O	1:B:178:THR:HA	2.08	0.52
1:A:142:VAL:O	1:A:178:THR:HA	2.10	0.52
1:A:443:VAL:HG12	1:A:494:PRO:CD	2.39	0.52
1:A:56:SER:HB2	1:A:143:SER:HB3	1.92	0.52
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.35	0.52
1:A:191:ILE:HG21	1:A:198:GLU:HB3	1.91	0.52
1:A:285:LEU:HB2	1:A:434:THR:HG21	1.92	0.51
1:B:64:ILE:HG22	1:B:65:ILE:HG22	1.92	0.51
1:B:325:LEU:HD23	1:B:335:PHE:HB2	1.91	0.51
1:B:316:ALA:HB3	1:B:348:CYS:HB3	1.92	0.51
1:B:148:THR:HG21	1:B:183:GLU:HG3	1.93	0.51
1:B:431:SER:O	1:B:437:ILE:HD11	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD22	1:A:472:ILE:HD13	1.93	0.51
1:B:483:PHE:HB3	1:B:486:PHE:HD2	1.75	0.51
1:B:219:THR:HB	1:B:234:GLU:HB3	1.93	0.50
1:A:305:ALA:HB2	1:A:374:ARG:CD	2.39	0.50
1:B:266:GLY:O	1:B:300:ARG:NH1	2.45	0.50
1:B:483:PHE:HB2	1:B:489:ILE:CD1	2.42	0.49
1:A:191:ILE:HD13	1:A:198:GLU:HG3	1.95	0.49
1:B:148:THR:HG22	1:B:182:THR:HG22	1.94	0.49
1:B:443:VAL:HG11	1:B:489:ILE:HG23	1.94	0.49
1:A:60:LEU:HD12	1:A:141:ARG:HB3	1.94	0.48
1:A:259:SER:CB	1:A:261:VAL:HG23	2.44	0.48
1:A:197:GLU:OE2	1:A:197:GLU:N	2.46	0.48
1:A:64:ILE:HG13	1:A:69:GLU:O	2.13	0.48
1:A:483:PHE:HB3	1:A:486:PHE:CD2	2.48	0.48
1:A:282:SER:HA	1:A:435:ASP:OD2	2.15	0.47
1:A:156:ALA:HB3	1:A:159:VAL:HG23	1.96	0.47
1:B:164:LEU:HG	1:B:200:VAL:HG11	1.97	0.47
1:B:191:ILE:HG21	1:B:198:GLU:HB3	1.95	0.47
1:B:54:LEU:HD13	1:B:90:PHE:CZ	2.49	0.47
1:A:76:PHE:CE2	1:A:150:VAL:HG21	2.50	0.46
1:B:378:ASP:HA	1:B:413:THR:OG1	2.16	0.46
1:A:317:TYR:HB3	1:A:351:PRO:HG3	1.97	0.46
1:B:483:PHE:HB2	1:B:489:ILE:HD11	1.95	0.46
1:A:266:GLY:O	1:A:300:ARG:NH2	2.47	0.46
1:A:203:ASN:HB3	1:A:225:LEU:CD2	2.46	0.46
1:B:436:THR:HG23	1:B:458:MET:HG2	1.98	0.46
1:B:432[B]:THR:O	1:B:459:ARG:NH2	2.49	0.46
1:B:60:LEU:CD2	1:B:141:ARG:HB3	2.45	0.45
1:B:382:ALA:O	1:B:385:ARG:CG	2.64	0.45
1:A:301:PHE:O	1:A:374:ARG:NH1	2.48	0.45
1:B:337:GLU:O	1:B:341:GLN:HG3	2.17	0.45
1:A:222:ILE:CG2	1:A:225:LEU:HG	2.47	0.44
1:B:58:GLN:HG3	1:B:92:TRP:CH2	2.53	0.44
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.82	0.44
1:A:43:LEU:HD11	1:A:182:THR:CG2	2.47	0.44
1:A:278:PHE:CD2	1:A:284:ILE:HD13	2.53	0.44
1:A:483:PHE:HB3	1:A:486:PHE:HD2	1.83	0.44
1:B:145:ASP:HA	1:B:146:SER:HA	1.73	0.44
1:B:90:PHE:HA	1:B:241:ASP:O	2.18	0.43
1:A:39:GLY:H	1:A:177:THR:CG2	2.16	0.43
1:B:58:GLN:HG3	1:B:92:TRP:HH2	1.82	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:HD3	1:A:278:PHE:O	2.18	0.43
1:B:21:MET:HE3	1:B:177:THR:HG21	2.01	0.43
1:B:52:LYS:HG2	1:B:181:THR:HG23	1.98	0.43
1:B:54:LEU:HD13	1:B:90:PHE:CE2	2.52	0.43
1:B:458:MET:HB2	1:B:463:HIS:CD2	2.53	0.43
1:B:365:SER:O	1:B:369:ASP:HB2	2.18	0.43
1:B:58:GLN:CG	1:B:92:TRP:HH2	2.32	0.43
1:B:469:GLU:HB2	1:B:483:PHE:CZ	2.53	0.43
1:A:76:PHE:CD2	1:A:150:VAL:CG2	3.02	0.43
1:A:54:LEU:HD13	1:A:90:PHE:CE2	2.54	0.42
1:A:156:ALA:HB3	1:A:159:VAL:CG2	2.49	0.42
1:A:245:ASN:HD22	1:A:245:ASN:HA	1.75	0.42
1:B:164:LEU:CD1	1:B:180:MET:HE1	2.43	0.42
1:A:37:PRO:HB2	1:A:203:ASN:HD21	1.84	0.42
1:A:259:SER:HB3	1:A:261:VAL:HG23	2.02	0.42
1:A:311:ARG:HA	1:A:343:LEU:O	2.19	0.42
1:A:280:LYS:HE3	1:A:407:GLU:O	2.20	0.42
1:B:21:MET:HB2	1:B:38:ILE:CD1	2.50	0.42
1:B:432[A]:THR:O	1:B:459:ARG:NH2	2.53	0.42
1:A:259:SER:HB2	1:A:261:VAL:HG23	2.01	0.41
1:B:61:TYR:CZ	1:B:65:ILE:HD13	2.55	0.41
1:B:351:PRO:HG2	1:B:382:ALA:HB1	2.01	0.41
1:A:285:LEU:HA	1:A:412:PHE:O	2.20	0.41
1:A:21:MET:CE	1:A:177:THR:CG2	2.92	0.41
1:B:443:VAL:HG12	1:B:494:PRO:HD3	2.02	0.41
1:B:164:LEU:HD23	1:B:197:GLU:HA	2.02	0.41
1:A:218:ARG:HH11	1:B:232:LYS:HE3	1.86	0.41
1:B:39:GLY:H	1:B:177:THR:CG2	2.34	0.41
1:B:144:ILE:HG22	1:B:147:VAL:HG22	2.02	0.41
1:B:224:LYS:HE2	1:B:224:LYS:HB3	1.98	0.41
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.81	0.41
1:A:222:ILE:HG21	1:A:225:LEU:HG	2.03	0.40
1:B:311:ARG:HB3	1:B:370:PHE:CE2	2.55	0.40
1:B:89:SER:OG	2:B:601:ATP:N6	2.52	0.40
1:B:60:LEU:HD22	1:B:141:ARG:HB3	2.02	0.40
1:B:311:ARG:HA	1:B:343:LEU:O	2.22	0.40
1:B:351:PRO:HB3	1:B:382:ALA:O	2.21	0.40
1:B:367:ILE:C	1:B:369:ASP:H	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:NZ	2:B:601:ATP:O3G[3_545]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	454/519 (88%)	420 (92%)	33 (7%)	1 (0%)	47	62
1	B	456/519 (88%)	426 (93%)	30 (7%)	0	100	100
All	All	910/1038 (88%)	846 (93%)	63 (7%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/444 (72%)	285 (89%)	36 (11%)	6	8
1	B	310/444 (70%)	267 (86%)	43 (14%)	3	4
All	All	631/888 (71%)	552 (88%)	79 (12%)	4	5

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	25	ILE
1	A	60	LEU
1	A	65	ILE
1	A	106	LEU
1	A	147	VAL
1	A	159	VAL
1	A	163	GLU
1	A	164	LEU
1	A	167	LEU
1	A	173	GLN
1	A	180	MET
1	A	187	GLU
1	A	193	ARG
1	A	222	ILE
1	A	224	LYS
1	A	245	ASN
1	A	260	ASN
1	A	269	ARG
1	A	294	LYS
1	A	318	GLU
1	A	319	GLU
1	A	323	GLN
1	A	352	GLU
1	A	356	LEU
1	A	357	GLU
1	A	360	LEU
1	A	361	GLN
1	A	364	LYS
1	A	397	ILE
1	A	424	SER
1	A	443	VAL
1	A	450	SER
1	A	451	ARG
1	A	471	MET
1	A	493	SER
1	B	25	ILE
1	B	30	ASP
1	B	38	ILE
1	B	50	THR
1	B	52	LYS
1	B	56	SER
1	B	65	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	75	THR
1	B	148	THR
1	B	163	GLU
1	B	183	GLU
1	B	187	GLU
1	B	196	VAL
1	B	200	VAL
1	B	216	ARG
1	B	224	LYS
1	B	261	VAL
1	B	270	LEU
1	B	314	LEU
1	B	318	GLU
1	B	319	GLU
1	B	321	ARG
1	B	323	GLN
1	B	348	CYS
1	B	352	GLU
1	B	356	LEU
1	B	357	GLU
1	B	360	LEU
1	B	362	ILE
1	B	364	LYS
1	B	369	ASP
1	B	374	ARG
1	B	385	ARG
1	B	397	ILE
1	B	400	THR
1	B	406	GLU
1	B	424	SER
1	B	430	ILE
1	B	434	THR
1	B	443	VAL
1	B	458	MET
1	B	471	MET
1	B	493	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	A	245	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	304	ASN
1	A	361	GLN
1	A	389	ASN
1	B	245	ASN
1	B	323	GLN
1	B	327	ASN
1	B	414	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ATP	A	602	3	26,33,33	0.66	0	31,52,52	0.73	1 (3%)
2	ATP	B	602	3	26,33,33	0.66	0	31,52,52	0.73	1 (3%)
2	ATP	B	601	3	26,33,33	0.66	0	31,52,52	0.89	2 (6%)
2	ATP	A	601	3	26,33,33	0.65	0	31,52,52	0.73	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	602	3	-	3/18/38/38	0/3/3/3
2	ATP	B	602	3	-	2/18/38/38	0/3/3/3
2	ATP	B	601	3	-	2/18/38/38	0/3/3/3
2	ATP	A	601	3	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ATP	C5-C6-N6	2.35	123.92	120.35
2	B	601	ATP	C5-C6-N6	2.33	123.89	120.35
2	B	602	ATP	C5-C6-N6	2.25	123.77	120.35
2	B	601	ATP	C3'-C2'-C1'	2.24	104.35	100.98
2	A	602	ATP	C5-C6-N6	2.22	123.72	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O1A
2	A	602	ATP	C5'-O5'-PA-O1A
2	A	601	ATP	C5'-O5'-PA-O3A
2	A	602	ATP	C5'-O5'-PA-O3A
2	A	601	ATP	PA-O3A-PB-O2B
2	B	601	ATP	PA-O3A-PB-O2B
2	A	601	ATP	C5'-O5'-PA-O2A
2	A	602	ATP	C5'-O5'-PA-O2A
2	B	601	ATP	PA-O3A-PB-O1B
2	B	602	ATP	PA-O3A-PB-O1B
2	A	601	ATP	PA-O3A-PB-O1B
2	B	602	ATP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

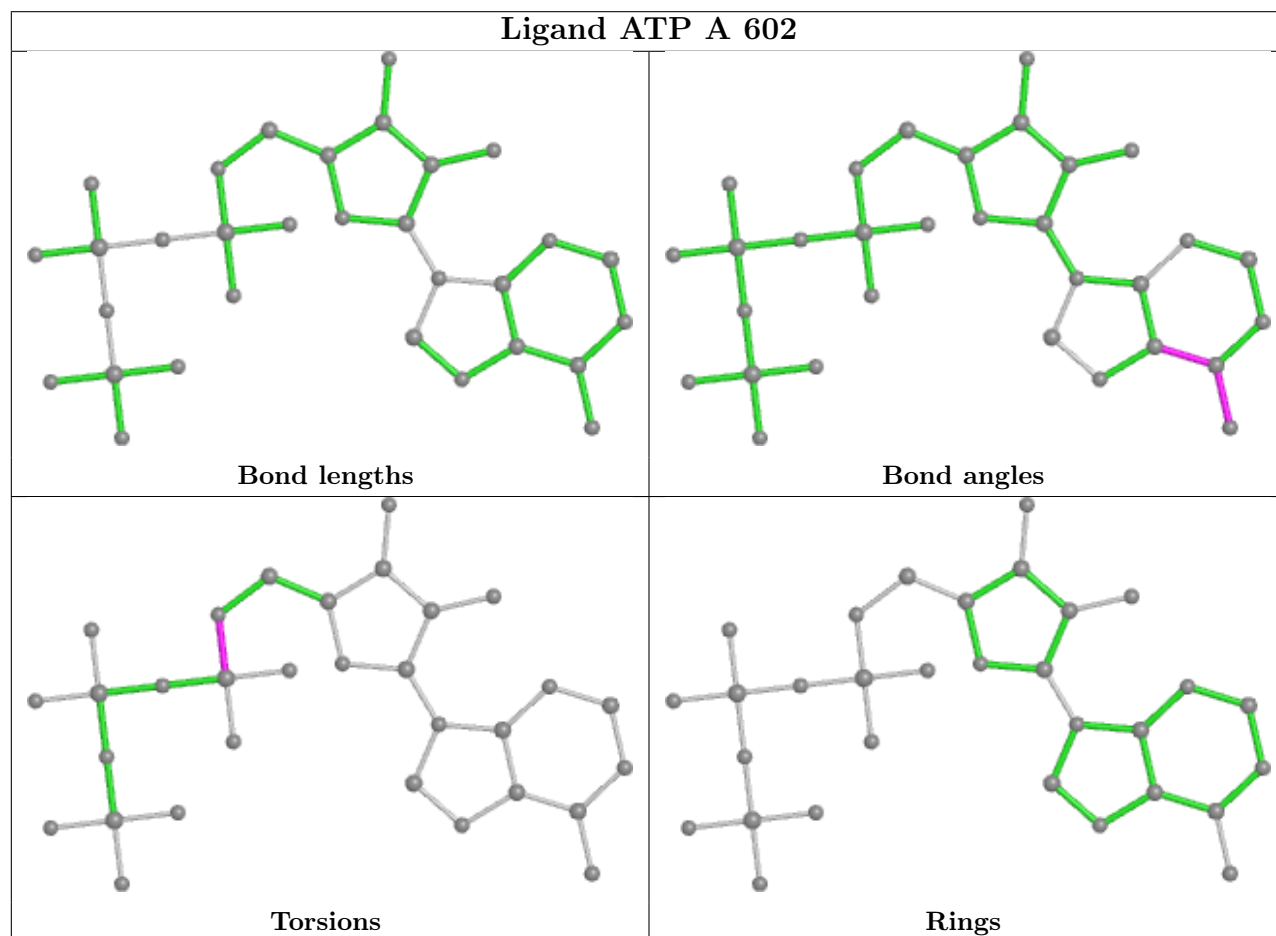
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ATP	1	1

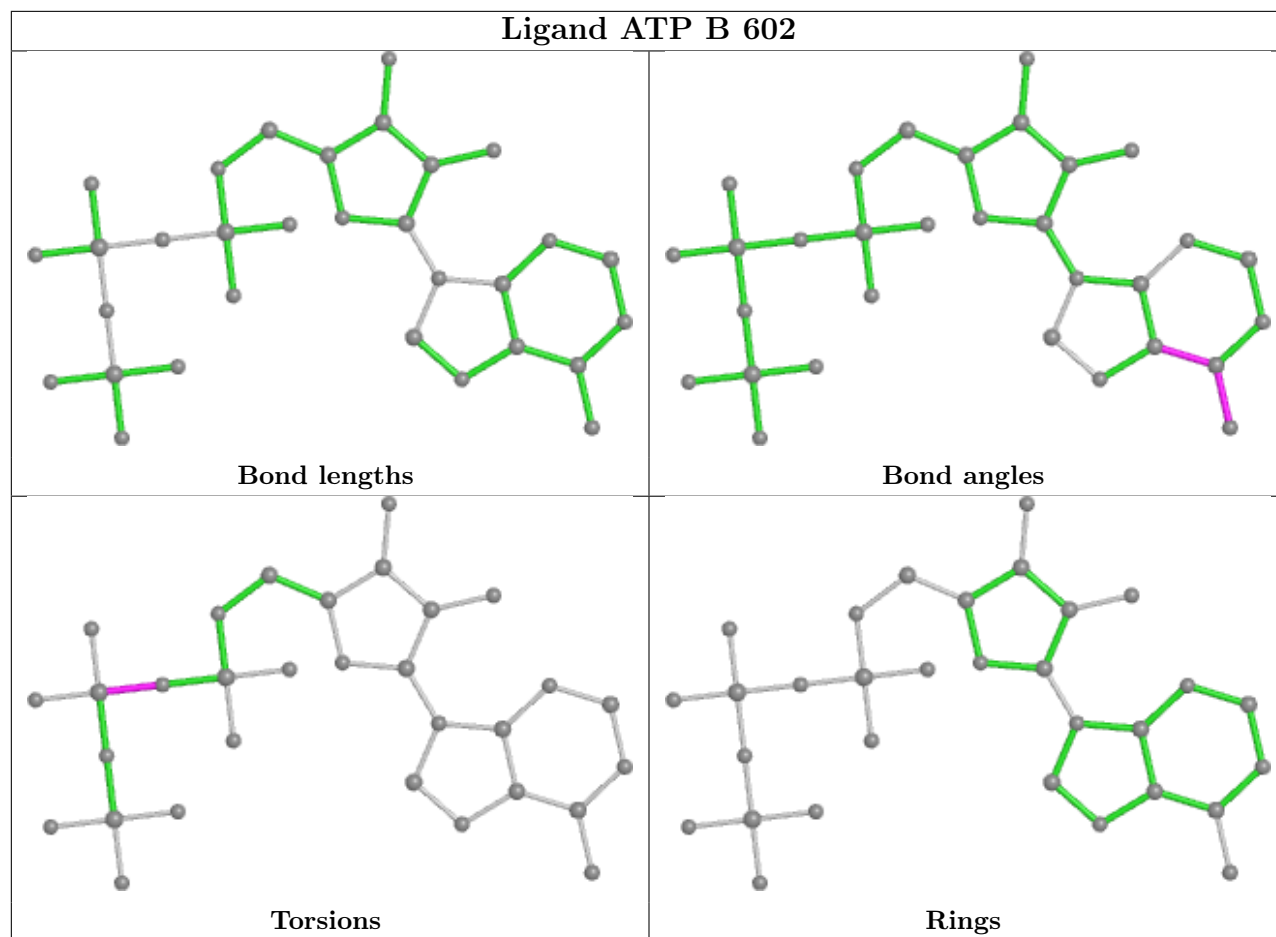
*Continued on next page...*

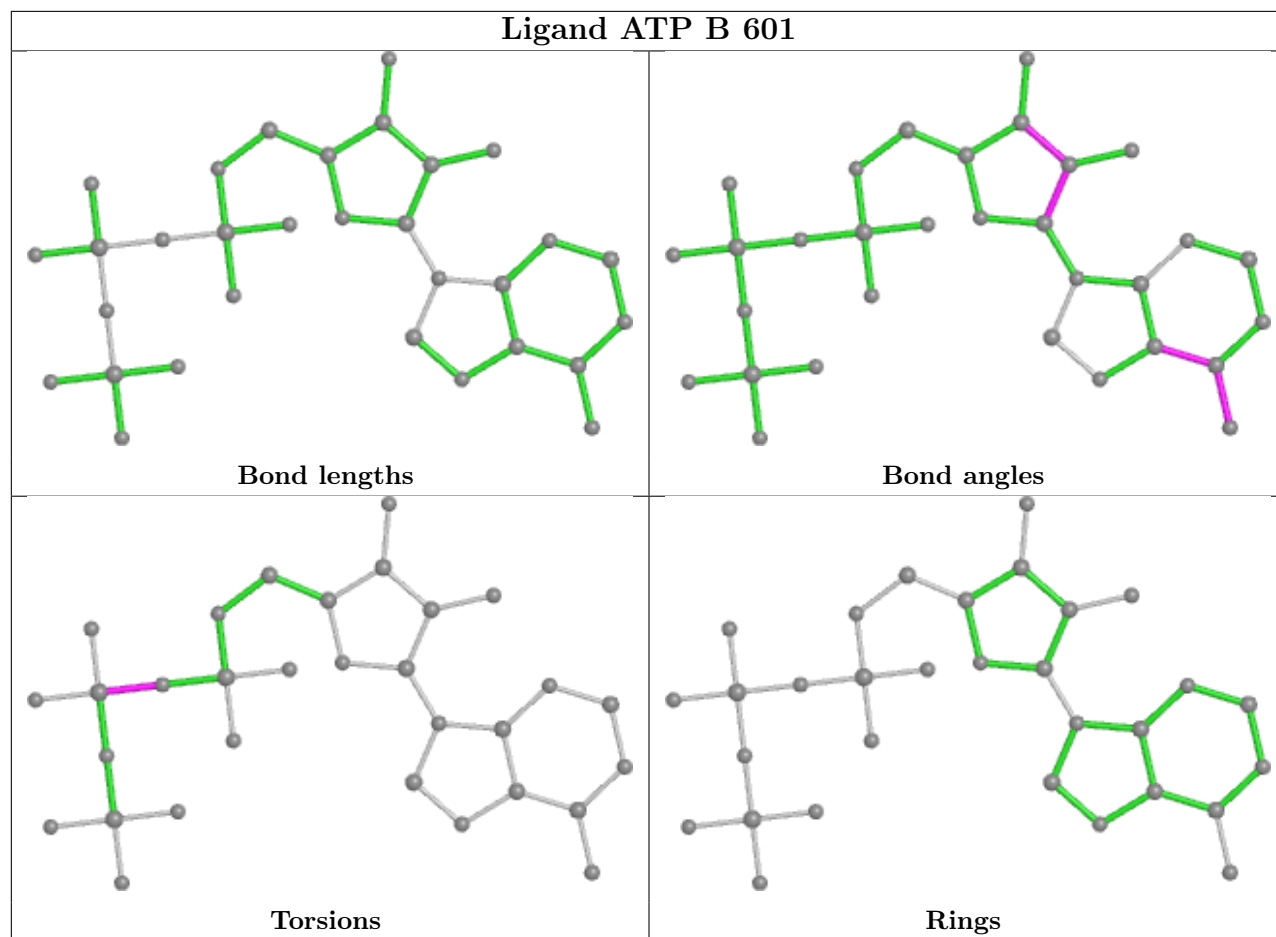
*Continued from previous page...*

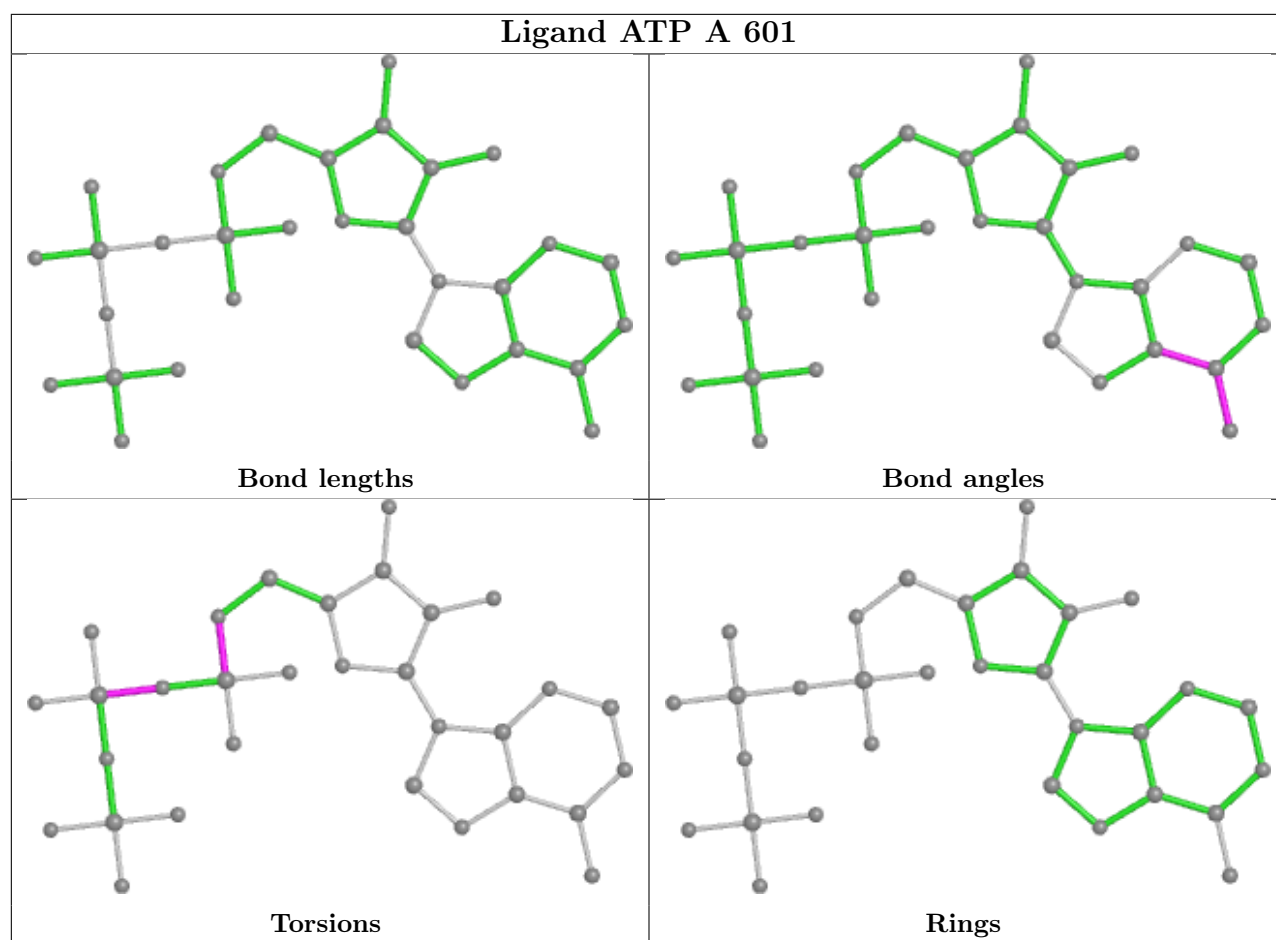
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	458/519 (88%)	0.44	35 (7%)	13 12	36, 57, 94, 108	0
1	B	460/519 (88%)	0.46	28 (6%)	21 20	34, 57, 95, 114	0
All	All	918/1038 (88%)	0.45	63 (6%)	16 15	34, 57, 95, 114	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	ALA	7.8
1	B	95	ALA	7.2
1	A	95	ALA	4.8
1	B	153	GLN	4.7
1	A	157	SER	4.5
1	B	94	LEU	3.9
1	B	106	LEU	3.8
1	A	92	TRP	3.7
1	A	276	GLY	3.6
1	A	123	LEU	3.5
1	A	179	VAL	3.4
1	B	99	ASP	3.4
1	A	135	GLN	3.3
1	B	44	VAL	3.3
1	A	258	SER	3.1
1	B	156	ALA	3.1
1	B	124	SER	2.9
1	A	163	GLU	2.9
1	A	159	VAL	2.8
1	B	126	LEU	2.8
1	A	136	LYS	2.8
1	B	81	GLN	2.7
1	A	158	SER	2.6
1	B	179	VAL	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	181	THR	2.6
1	B	169	ALA	2.6
1	B	24	MET	2.6
1	A	91	GLY	2.6
1	A	153	GLN	2.6
1	B	241	ASP	2.5
1	B	163	GLU	2.5
1	A	173	GLN	2.5
1	B	369	ASP	2.4
1	A	284	ILE	2.4
1	B	256	GLN	2.4
1	B	34	GLY	2.4
1	B	182	THR	2.4
1	A	138	ARG	2.3
1	A	143	SER	2.3
1	B	143	SER	2.3
1	B	43	LEU	2.3
1	B	155	ASP	2.3
1	B	353	SER	2.3
1	B	154	TYR	2.3
1	A	436	THR	2.2
1	B	329	TYR	2.2
1	A	180	MET	2.2
1	A	104	PHE	2.2
1	B	90	PHE	2.2
1	A	369	ASP	2.2
1	B	411	LEU	2.2
1	A	190	PRO	2.1
1	A	147	VAL	2.1
1	B	52	LYS	2.1
1	A	145	ASP	2.1
1	A	405	GLN	2.1
1	A	101	GLY	2.1
1	A	132	TYR	2.0
1	A	137	TYR	2.0
1	A	59	PHE	2.0
1	A	269	ARG	2.0
1	A	82	ASP	2.0
1	A	52	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

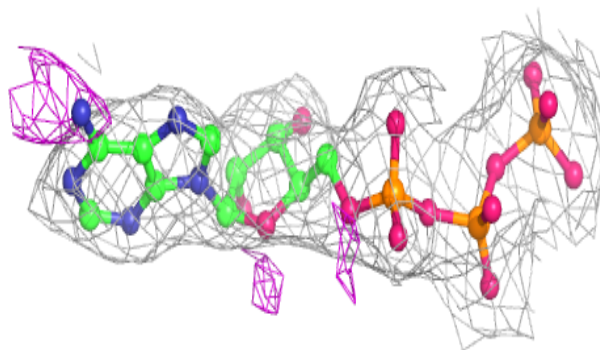
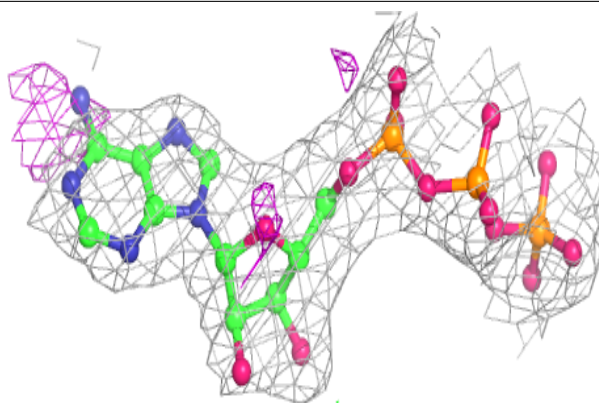
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ATP	A	601	31/31	0.89	0.16	49,51,53,53	0
3	MG	B	603	1/1	0.91	0.05	51,51,51,51	0
2	ATP	B	601	31/31	0.92	0.14	48,53,58,58	0
2	ATP	B	602	31/31	0.93	0.13	38,39,46,47	0
3	MG	B	604	1/1	0.93	0.14	42,42,42,42	0
2	ATP	A	602	31/31	0.94	0.12	37,38,46,46	0
3	MG	A	603	1/1	0.96	0.15	50,50,50,50	0
3	MG	A	604	1/1	0.97	0.05	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

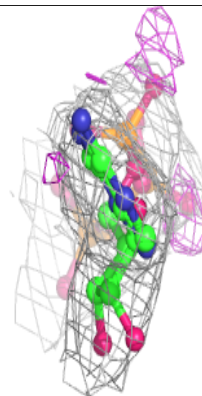
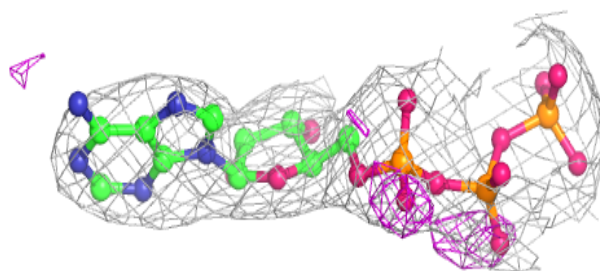
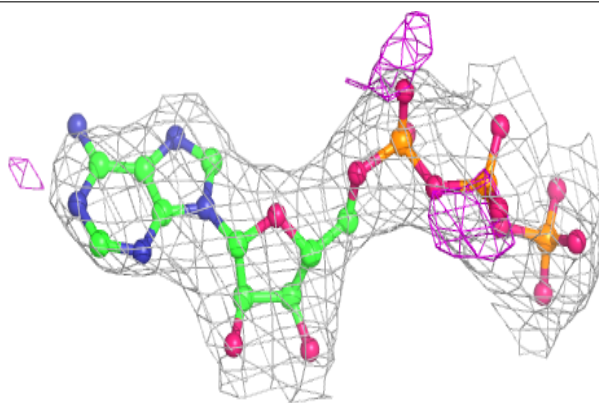


**Electron density around ATP A 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

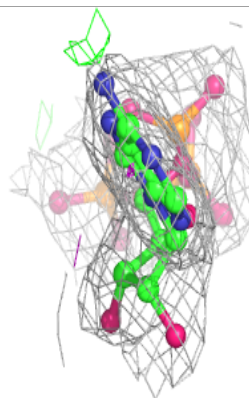
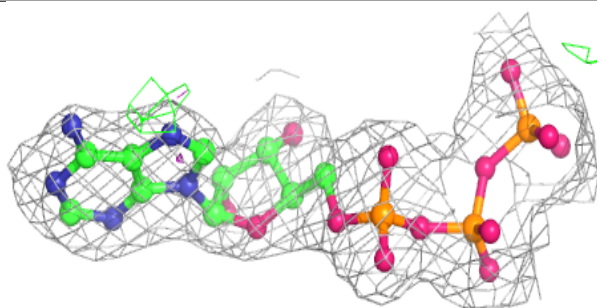
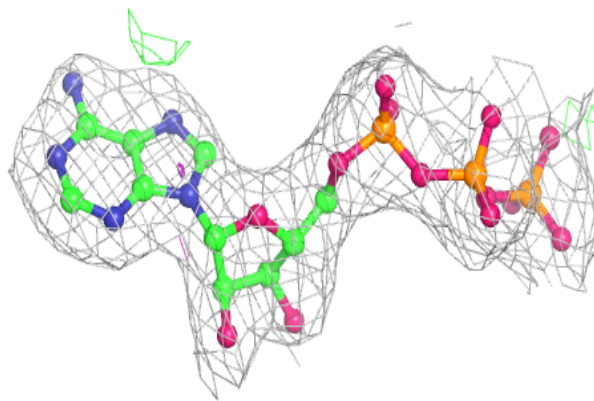
**Electron density around ATP B 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

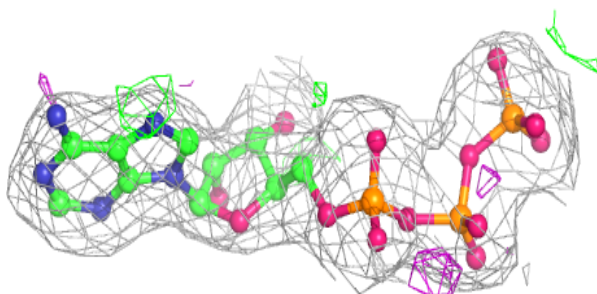
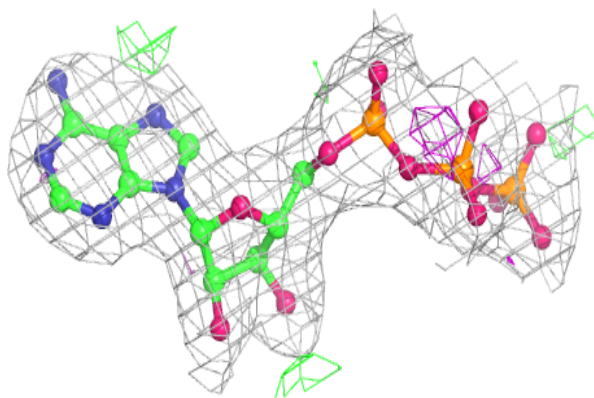


**Electron density around ATP B 602:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ATP A 602:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.